Deriving the static interaction between electric dipoles via the quantum gauge transformation

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Abstract

Gauge transformation leaves the electric and the magnetic fields unchanged as long as the gauge function is treated classically. In this paper we consider the gauge transformation commonly used to obtain the electric dipole interaction Hamiltonian in a system of dipoles and the electromagnetic field (Göppert-Mayer transformation) and treat the vector potential that appear in the gauge function as an operator. While it modifies the electric field, the static interaction between the dipoles is derived.

1 Introduction

In the standard textbooks of quantum mechanics and electromagnetism, A: the notion of gauge transformation is introduced before fields are quantized so that the gauge function is treated classically, and B: only time-varying fields are considered in the field quantization. Derivation of the static force between charges or dipoles in the quantum regime, i.e., as a result of the exchange of virtual photons between them requires some amount of knowledges on the quantum field theory[1]. In this paper, we take up the Göppert-Mayer transformation and perform the transformation while treating the vector potential that appear in this transformation as an operator. As a conseqence of this "quantum" transformation, it is shown that the static interaction between the dipoles emerges and the static dipole-field is added to the electric field operator.

2 Göppert-Mayer transformation

Consider an atom consists of an electron of charge $-e$ orbiting around an nucleus of charge $+e$ fixed at the origin. The electron is also interacting with the external electromagnetic field in addition to the Coulomb field created by the nucleus. We choose Coulomb gauge ($\phi = 0$) for the external electromagnetic field. Then the Schrödinger equation for the electron is written as

$$i\hbar \frac{\partial}{\partial t}|\varphi\rangle = \left\{ \frac{1}{2m}[\boldsymbol{p} + e\boldsymbol{A}(\boldsymbol{r}, t)]^2 + V(\boldsymbol{r}) \right\} |\varphi\rangle \tag{1}$$

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where $V(\boldsymbol{r})$ is the Coulomb potential created by the nucleus. In the long wavelength approximation, the value of the vector potential $\boldsymbol{A}(\boldsymbol{r},t)$ is approximated by $\boldsymbol{A}(\boldsymbol{0},t)$, so that (1) becomes

$$i\hbar\frac{\partial}{\partial t}|\varphi\rangle = \left\{\frac{1}{2m}[\boldsymbol{p}+e\boldsymbol{A}(\boldsymbol{0},t)]^2+V(\boldsymbol{r})\right\}|\varphi\rangle. \tag{2}$$

The Göppert-Mayer transformation[2] is a gauge transformation using the gauge function

$$\chi(\boldsymbol{r},t) = -\boldsymbol{r}\cdot\boldsymbol{A}(\boldsymbol{0},t),$$

that transforms the state $|\varphi\rangle$ to $|\tilde{\varphi}\rangle = T|\varphi\rangle$ with a unitary transformation $T=\exp(-i\frac{e}{\hbar}\chi(\boldsymbol{r},t)) = \exp(-\frac{i}{\hbar}\boldsymbol{d}\cdot\boldsymbol{A}(\boldsymbol{0},t))$ where $\boldsymbol{d}=-e\boldsymbol{r}$ is the dipole moment of the atom. Substituting $|\varphi\rangle = T^{-1}|\tilde{\varphi}\rangle$ into (2), or by first writing (2) in the gauge independent form and then using the relation $\tilde{\boldsymbol{A}}(\boldsymbol{r},t)=\boldsymbol{A}(\boldsymbol{r},t)+\nabla\chi(\boldsymbol{r},t)$ and $\tilde{\phi}(\boldsymbol{r},t)=\phi(\boldsymbol{r},t)-\partial_t\chi(\boldsymbol{r},t)$, an equation for $|\tilde{\varphi}\rangle$ is obtained:

$$i\hbar\frac{\partial}{\partial t}|\tilde{\varphi}\rangle = \left\{\frac{1}{2m}\boldsymbol{p}^2+V(\boldsymbol{r})-\boldsymbol{d}\cdot\boldsymbol{E}(\boldsymbol{0},t)\right\}|\tilde{\varphi}\rangle. \tag{3}$$

Here we also used the relation $\boldsymbol{E}(\boldsymbol{r},t)=-\partial_t\boldsymbol{A}(\boldsymbol{r},t)$ applicable for the Coulomb gauge. The Göppert-Mayer transformation has an aspect that it rewrites the Hamiltonian into a standard form, i.e., as a sum of the kinetic energy and the potential energy.

3 Transformation in the quantum regime

In deriving (3), we implicitly assumed that $\partial_t T = -i\frac{e}{\hbar}T\partial_t\chi(\boldsymbol{r},t)$ which holds no longer if $\chi(\boldsymbol{r},t)$ is an operator-valued function. Now we consider n atoms interacting with the electromagnetic field, and perform the transformation in the quantum regime. The Schrödinger equation in the long wavelength approximation is written as

$$i\hbar\frac{\partial}{\partial t}|\varphi\rangle = \sum_q\left\{\frac{1}{2m}[\boldsymbol{p}_q+e\boldsymbol{A}(\boldsymbol{R}_q,t)]^2+V(\boldsymbol{r}_q-\boldsymbol{R}_q)\right\}|\varphi\rangle \tag{4}$$

where $\boldsymbol{r}_q$ ($\boldsymbol{R}_q$) is the position of the electron (nucleus) of the qth atom. The unitary transformation T on the state as $|\tilde{\varphi}\rangle = T|\varphi\rangle$ is now given by $T=\exp(-\frac{i}{\hbar}\sum_q\boldsymbol{d}_q\cdot\boldsymbol{A}(\boldsymbol{R}_q,t))$ where $\boldsymbol{d}_q=-e(\boldsymbol{r}_q-\boldsymbol{R}_q)$ is the dipole moment of the qth atom. We shall rewrite (4) in terms of $|\tilde{\varphi}\rangle = T|\varphi\rangle$ and $\tilde{\boldsymbol{E}}(\boldsymbol{r},t)=T\boldsymbol{E}(\boldsymbol{r},t)T^\dagger$ while treating $\boldsymbol{A}(\boldsymbol{r},t)$ as an operator (if $\boldsymbol{A}(\boldsymbol{r},t)$ is treated as a classical quantity, then we obtain just a set of n equations each equivalent to (3)). It is readily shown that $|\tilde{\varphi}\rangle$ obeys

$$i\hbar\frac{\partial}{\partial t}|\tilde{\varphi}\rangle = \left\{\sum_q\left[\frac{1}{2m}\boldsymbol{p}_q^2+V(\boldsymbol{r}_q-\boldsymbol{R}_q)\right]-i\hbar T(\partial_t T^{-1})\right\}|\tilde{\varphi}\rangle. \tag{5}$$

Writing T as $T = e^X$ with $X = -\frac{i}{\hbar}\sum_q \boldsymbol{d}_q \cdot \boldsymbol{A}(\boldsymbol{R}_q, t)$ and going back to the definition of the exponential $e^X = \lim_{m\to\infty}\left(1+\frac{X}{m}\right)^m$, it is shown that $T\partial_t T^{-1}$ can be written generally as

$$T\partial_t T^{-1} = \int_0^1 ds\, e^{sX} Y e^{-sX} = \int_0^1 ds\, T_s Y T_{-s}$$

where $Y = \partial_t X = \frac{i}{\hbar}\sum_q \boldsymbol{d}_q \cdot \boldsymbol{E}(\boldsymbol{R}_q, t)$ and $T_s = e^{sX}$. Define a function $f(s)$ as $f(s) = T_s Y T_{-s}$. Then

$$f'(s) = T_s[X, Y]T_{-s} = [X, Y] \tag{6}$$

using the fact that $[X, Y]$ commutes with X in our system as will be shown below. Solving (6) as

$$T_s Y T_{-s} = f(s) = Y + s[X, Y] \tag{7}$$

which leads to

$$T\partial_t T^{-1} = \int_0^1 ds\, f(s) = Y + \frac{1}{2}[X, Y] = T_{\frac{1}{2}} Y T_{-\frac{1}{2}} = \tilde{Y} - \frac{1}{2}[X, Y]$$

with $\tilde{Y} = TYT^{-1}$. Now we expand $[X, Y]$:

$$[X, Y] = \frac{1}{\hbar^2}\sum_{qq'}\sum_{m\,m'} d_{q\,m} d_{q'm'}[A_m(\boldsymbol{R}_q, t), E_{m'}(\boldsymbol{R}_{q'}, t)].$$

The general commutation relation between the vector potential operator and the electric field operator is given by (24) and (27) of COMPLEMENT $\mathrm{C_{III}}$ of [3] (p.226-7). From this, the simultaneous commutation relation is calculated as

$$[A_m(\boldsymbol{R}, t), E_{m'}(\boldsymbol{R}', t)] = \frac{i\hbar}{4\pi\epsilon_0}\frac{1}{\rho^3}\left(\delta_{mm'} - 3\,\hat{\rho}_m\hat{\rho}_{m'}\right) \tag{8}$$

where $\boldsymbol{\rho} = \boldsymbol{R} - \boldsymbol{R}'$, $\rho = |\boldsymbol{\rho}|$, and $\hat{\boldsymbol{\rho}} = \frac{\boldsymbol{\rho}}{\rho}$ (we omit here the term proportional to $\delta(\boldsymbol{\rho})$). Note that the right-hand side of the above equation is a c-number. Finally putting all togther into (5), we obtain

$$i\hbar\frac{\partial}{\partial t}|\tilde{\varphi}\rangle = \left\{ H_0 + H_{ext} + \sum_{q>q'} \epsilon_{dip}(\boldsymbol{R}_q - \boldsymbol{R}_{q'}, \boldsymbol{d}_q, \boldsymbol{d}_{q'}) + \epsilon_{self} \right\}|\tilde{\varphi}\rangle, \tag{9}$$

with $H_0 = \sum_q \left\{\frac{1}{2m}\boldsymbol{p}_q^2 + V(\boldsymbol{r}_q - \boldsymbol{R}_q)\right\}$, $H_{ext} = -\sum_q \boldsymbol{d}_q \cdot \tilde{\boldsymbol{E}}(\boldsymbol{R}_q, t)$,

$$\epsilon_{dip}(\boldsymbol{R}, \boldsymbol{d}, \boldsymbol{d}') = \frac{1}{4\pi\epsilon_0}\frac{1}{R^3}\{\boldsymbol{d}\cdot\boldsymbol{d}' - 3(\boldsymbol{d}\cdot\hat{\boldsymbol{R}})(\boldsymbol{d}'\cdot\hat{\boldsymbol{R}})\},$$

and $\epsilon_{self} = \frac{1}{2}\sum_q \epsilon_{dip}(\boldsymbol{0}, \boldsymbol{d}_q, \boldsymbol{d}_q)$ is the dipole self energy which is singular. The ϵ_{dip} terms describe the static interaction between different dipoles where as H_{ext}

corresponds to the electric dipole interaction with the external field. Redefining Y as $Y = \boldsymbol{E}(\boldsymbol{R}, t)$ and using the relation (7), $\tilde{\boldsymbol{E}}(\boldsymbol{R}, t)$ is calculated as

$$\tilde{\boldsymbol{E}}(\boldsymbol{R}, t) = TYT^\dagger = T_1 Y T_{-1} = Y + [X, Y].$$

Again using the commutation relation (8), the relation between the electric field operators before and after the gauge transformation is calculated as

$$\boldsymbol{E}(\boldsymbol{R}, t) = \tilde{\boldsymbol{E}}(\boldsymbol{R}, t) + \sum_q \boldsymbol{E}_{dip}(\boldsymbol{R} - \boldsymbol{R}_q, \boldsymbol{d}_q)$$

where

$$\boldsymbol{E}_{dip}(\boldsymbol{R}, \boldsymbol{d}) = -\frac{1}{4\pi\epsilon_0}\frac{1}{R^3}\left\{\boldsymbol{d} - 3(\boldsymbol{d}\cdot\hat{\boldsymbol{R}})\hat{\boldsymbol{R}}\right\} \tag{10}$$

is the electric field created by a dipole of dipole moment $\boldsymbol{d}$ at the distance $\boldsymbol{R}$. We see that the electric field operators in the two pictures differ by the electric field created by n dipoles.

4 Conclusion and discussion

By treating the gauge function of the Göppert-Mayer transformation as an operator, the static interaction between the dipoles is derived. Let us call the picture before (after) the transformation P1 (P2). It is noted that, in P2, the static dipole interaction term is present even in the absence of photons. Going back to P1, the corresponding state contains (virtual) photons which yield forces between the dipoles.

A Coulomb potential

In this appendix we look for a unitary transformation T which leads to the Coulomb potential:

$$\boldsymbol{E}(\boldsymbol{r}, t) = \tilde{\boldsymbol{E}}(\boldsymbol{r}, t) + \boldsymbol{E}_c(\boldsymbol{r})$$

where $\tilde{\boldsymbol{E}}(\boldsymbol{r}, t) = T\boldsymbol{E}(\boldsymbol{r}, t)T^\dagger$ and $\boldsymbol{E}_c(\boldsymbol{r}) = \frac{q}{4\pi\epsilon_0}\frac{\boldsymbol{r}}{r^3} = -\nabla\phi_c(r)$ is the electric field derived from the Coulomb potential $\phi_c(r) = \frac{q}{4\pi\epsilon_0}\frac{1}{r}$. The relation

$$\begin{aligned}\boldsymbol{E}_{dip}(\boldsymbol{r} - \boldsymbol{s}, -q\,d\boldsymbol{s}) &= \frac{q}{4\pi\epsilon_0}\frac{1}{|\boldsymbol{r}-\boldsymbol{s}|^3}\left\{d\boldsymbol{s} - 3\frac{[d\boldsymbol{s}\cdot(\boldsymbol{r}-\boldsymbol{s})](\boldsymbol{r}-\boldsymbol{s})}{|\boldsymbol{r}-\boldsymbol{s}|^2}\right\} \\ &= -(d\boldsymbol{s}\cdot\nabla_{\boldsymbol{s}})\boldsymbol{E}_c(\boldsymbol{r} - \boldsymbol{s})\end{aligned}$$

(see (10)) suggests to use $T = \exp(\frac{i}{\hbar}q\int_{\boldsymbol{0}}\boldsymbol{A}(\boldsymbol{s}, t)\cdot d\boldsymbol{s})$ (instead of $T = \exp(-\frac{i}{\hbar}\boldsymbol{d}\cdot\boldsymbol{A}(\boldsymbol{0}, t))$ of the Göppert-Mayer transformation) where the integration path goes from the origin to somewhere infinity (imagine a chain of dipoles that connects the origin to infinity). T itself depends on the integration path, but $\tilde{\boldsymbol{E}}$ does not as we shall see. Again writing T as $T = e^X$ with $X = \frac{i}{\hbar}q\int_{\boldsymbol{0}}\boldsymbol{A}(\boldsymbol{s}, t)\cdot d\boldsymbol{s}$ and defining Y as $Y = E_m(\boldsymbol{r}, t)$, then (7) leads to

$$\tilde{E}_m(\boldsymbol{r}, t) = f(1) = X + [X, Y]. \tag{11}$$

Using the simultaneous commutation relation (8) in the form

$$\begin{aligned}[A_{m'}(\boldsymbol{s},t), E_m(\boldsymbol{r},t)] &= \tfrac{i\hbar}{4\pi\epsilon_0}\tfrac{1}{\rho^3}\left(\delta_{mm'} - 3\,\hat{\rho}_m\hat{\rho}_{m'}\right) \\ &= \tfrac{i\hbar}{4\pi\epsilon_0}\tfrac{\partial}{\partial\rho_{m'}}\tfrac{\rho_m}{\rho^3}\end{aligned} \tag{12}$$

where $\boldsymbol{\rho} = \boldsymbol{s} - \boldsymbol{r}$, $\rho = |\boldsymbol{\rho}|$, and $\hat{\boldsymbol{\rho}} = \frac{\boldsymbol{\rho}}{\rho}$, $[X, Y]$ is calculated as

$$\begin{aligned}[X, Y] &= \tfrac{i}{\hbar}q\int_{\boldsymbol{0}}\textstyle\sum_{m'}[A_{m'}(\boldsymbol{s},t), E_m(\boldsymbol{r},t)]ds_{m'} \\ &= \tfrac{i}{\hbar}q\int_{\boldsymbol{0}}\textstyle\sum_{m'}\tfrac{i\hbar}{4\pi\epsilon_0}\tfrac{\partial}{\partial s_{m'}}\tfrac{s_m - r_m}{|\boldsymbol{s}-\boldsymbol{r}|^3}ds_{m'} \\ &= -\tfrac{q}{4\pi\epsilon_0}\int_{\boldsymbol{0}}d\boldsymbol{s}\cdot\nabla_{\boldsymbol{s}}\tfrac{s_m - r_m}{|\boldsymbol{s}-\boldsymbol{r}|^3} \\ &= -\tfrac{q}{4\pi\epsilon_0}\tfrac{r_m}{r^3}.\end{aligned}$$

Substituting this into (11) we obtain

$$\tilde{\boldsymbol{E}}(\boldsymbol{r},t) = \boldsymbol{E}(\boldsymbol{r},t) - \frac{q}{4\pi\epsilon_0}\frac{\boldsymbol{r}}{r^3}$$

as expected.

References

[1] Zee, A.: Quantum Field Theory in a Nutshell, Princeton University Press (2003)

[2] Göppert-Mayer, G., Ann. Phys., 401, 273 (1931)

[3] Cohen-Tannoudji, C., Dupont-Roc, J., Grynberg, G.: Photons and Atoms, John Wiley and Sons (1987)